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A first-principle study on the properties of a new series of quaternary Heusler alloys CoFeScZ (Z=P, As, Sb)

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ABSTRACT

The electronic structures and magnetic properties of a new series of quaternary Heusler alloys CoFeScZ (Z=P, As, Sb) are investigated through first-principle calculations. CoFeScP is found to have half-metallic ferromagnetism with a large half-metallic gap of 0.60 eV. The results show that both CoFeScAs and CoFeScSb are nearly half-metal under the equilibrium lattice constants. The change of the properties of CoFeScAs and CoFeScSb with pressure is investigated.

1. Introduction

As is known, searching for semiconductor with half-metallic (HM) ferromagnetism is of importance to the development of spintronics. Since the prediction of HM ferromagnetism of Heusler alloy NiMnSb by first-principle calculations in 1983 [1], HM ferromagnetism has attracted great interest. As Heusler alloys show excellent properties with high Curie temperature and 100% spin polarization at Fermi level, these alloys are good for spintronic devices. With great effort studying on Heusler alloys, a lot of these alloys and many novel properties have been discovered [2–4].

As described in Refs. [5–14,16,17], the so-called full-Heusler compounds consist of two transition metallic or rare-earth elements and one main group element with a formula X_2YZ. They crystallize either in the Cu_2MnAl structure ($L2_1$, space group No. 225, Fm $\bar{3}$ m), or in the Hg_2CuTi structure (space group No.216, F $\bar{4}$ 3m). In recent reports [18–24], the full-Heusler compounds would form the so-called LiMgPdSn or Y-type structure [25] (space group No. 216, F $\bar{4}$ 3m) Heusler compound if one of the X occupations is replaced by a different transition metal. The new style Heusler has a stoichiometry of 1:1:1:1 for X_1, X_2, Y and Z elements. Till now only the CoFeYZ (Y=Mn, Cr, V, Ti; Z=Al, Si, Ga, Ge, Sb) has been investigated. The results show that CoFeMnZ (Z=Al, Si, Ga, Ge), NiFeMnGa, NiCoMnGa, CoFeCrZ (Z=Al, Si, Ga, Ge), CoFeTiZ (Z=Si, Ge, As, Sb) and CoFeVZ (Z=Ge, As, Sb) have HM ferromagnetism under the equilibrium lattice constant [18–24]. It is pity that among these Heusler alloys only CoFeMnSi, CoFeCrZ (Z=Al, Si), CoFeTiZ (Z=Si, As) and CoFeVSb have wide enough gaps. It should be noticed that only with a wide enough gap the HM ferromagnetism of the Heusler alloys may probably be stable when the external conditions change near the ground state.

Inspired by the above investigations, we calculated a new series of quaternary Heusler alloys with the formula CoFeScZ (Z=P, As, Sb). The results show that the magnetic moment of CoFeScP, CoFeScAs and CoFeScSb is 1.00 μ_B, 1.01 μ_B and 1.02 μ_B respectively under the equilibrium lattice constant. CoFeScP has HM ferromagnetism with a large wide gap of 0.60 eV under the equilibrium lattice constant. CoFeScAs and CoFeScSb are close to have HM ferromagnetism under the equilibrium lattice constant. Finally the effect of pressure on the properties of CoFeScAs and CoFeScSb is studied. The results show that while applying appropriate pressure, CoFeScAs and CoFeScSb exhibit HM ferromagnetism with wide enough gaps.

2. Computational method

The lattice optimization, the electronic density of states (DOS), the magnetic moment and the band structure of CoFeScZ (Z=P, As, Sb) are calculated by using the full-potential local-orbital minimum-basis band structure scheme (FPLO) with generalized gradient approximation (GGA) [26–28]. For the irreducible Brillouin zone, we use the k meshes of $20 \times 20 \times 20$ for all the calculations. The convergence criteria of self-consistent iterations are set to 10^{-6} to the density and 10^{-8} Hartree to the total energy per

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Table 1
The occupations of the three types of quaternary Heusler alloys CoFeScZ (Z=P, As, Sb) for the atoms of every lattice.

Type	4a (0,0,0)	4c ($\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$)	4b ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$)	4d ($\frac{3}{4}$, $\frac{3}{4}$, $\frac{3}{4}$)
Y-type (I)	Z	Fe	Sc	Co
Y-type (II)	Z	Sc	Fe	Co
Y-type (III)	Fe	Z	Sc	Co

Table 2
The results of the lattice optimization of the quaternary Heusler alloys CoFeScZ. L_{opt} is the equilibrium lattice constant. E_{tot} and m_{tot} are the total energy and magnetic moment respectively. E_g represents the band gap near the Fermi energy.

Compound	L_{opt} (Å)	E_{tot} (Ry)	m_{tot} (μ_B)	E_g (eV)	Half-metallicity
CoFeScP					
Type (I)	5.789	−1886.33596	1.00	0.60	Yes
Type (II)	6.003	−1886.32095	3.54	0	No
Type (III)	6.003	−1886.32306	3.61	0	No
CoFeScAs					
Type (I)	5.942	−2845.82708	1.01	0	Nearly
Type (II)	6.149	−2845.81568	3.56	0	No
Type (III)	6.156	−2845.81711	3.67	0	No
CoFeScSb					
Type (I)	6.198	−4957.09817	1.02	0	Nearly
Type (II)	6.391	−4957.07953	3.55	0	No
Type (III)	6.404	−4957.07860	3.73	0	No

Table 3
The partial magnetic moments of the Heusler alloys CoFeScZ (Z=P, As, Sb) in type (I) under the equilibrium lattice constant.

Compound	m_Z (μ_B)	m_{Fe} (μ_B)	m_{Sc} (μ_B)	m_{Co} (μ_B)	m_{tot} (μ_B)
PFeScCo	−0.01	0.67	−0.18	0.52	1.00
AsFeScCo	−0.01	0.72	−0.21	0.51	1.01
SbFeScCo	−0.04	0.81	−0.26	0.51	1.02

formula unit.

According to the symmetry, the quaternary Heusler alloys have three kinds of lattice structures. For CoFeScZ (Z=P, As, Sb), the occupations are determined in consistent with the method of the previous work [18–22,24] shown in Table 1. The space group of the lattice is No. 216, F $\bar{4}$ 3m which is called Y-type or LiMgPdSn structure.

3. Results and discussions

The calculation results of the lattice optimization which use total energy as a function are shown in Table 2. From Table 2, we can get that the energy of Y-type (I) structure is the lowest among the three. And this structure alloy exhibits half-metallicity which is consistent with the previous articles [18–22,24]. Table 3 shows the partial and total magnetic moment of CoFeScP, CoFeScAs and CoFeScSb under the equilibrium lattice constant.

As is shown in Table 2, the magnetic moment of CoFeScP, CoFeScAs and CoFeScSb are 1.00 μ_B, 1.01 μ_B and 1.02 μ_B respectively under the equilibrium lattice constant. So the total magnetic moment of CoFeScP, CoFeScAs and CoFeScSb is 1.00 μ_B or close to be 1.00 μ_B. There are 25 valence electrons in CoFeScZ (Z=P, As and Sb), and the total magnetic moment of 1 μ_B per formula unit obeys the Slater–Pauling behavior of HM ferromagnets with Heusler structure [29–31]:

$$M_{tot} = (Z_{tot} - 24)\mu_B \quad (1)$$

where Z_{tot} and M_{tot} are the number of total valence electrons and the total magnetic moment respectively. As is shown in Table 3, the values of magnetic moment of Fe atoms are 0.67 μ_B, 0.72 μ_B and 0.81 μ_B for CoFeScP, CoFeScAs and CoFeScSb respectively. And the values of magnetic moment of Co atoms are 0.52 μ_B, 0.51 μ_B and 0.51 μ_B for CoFeScP, CoFeScAs and CoFeScSb respectively. So, the magnetic interactions are ferromagnetic between Co and Fe atoms in CoFeScP, CoFeScAs and CoFeScSb.

As is shown in Table 2, CoFeScP has HM ferromagnetism with a large wide band gap of 0.60 eV under the equilibrium lattice

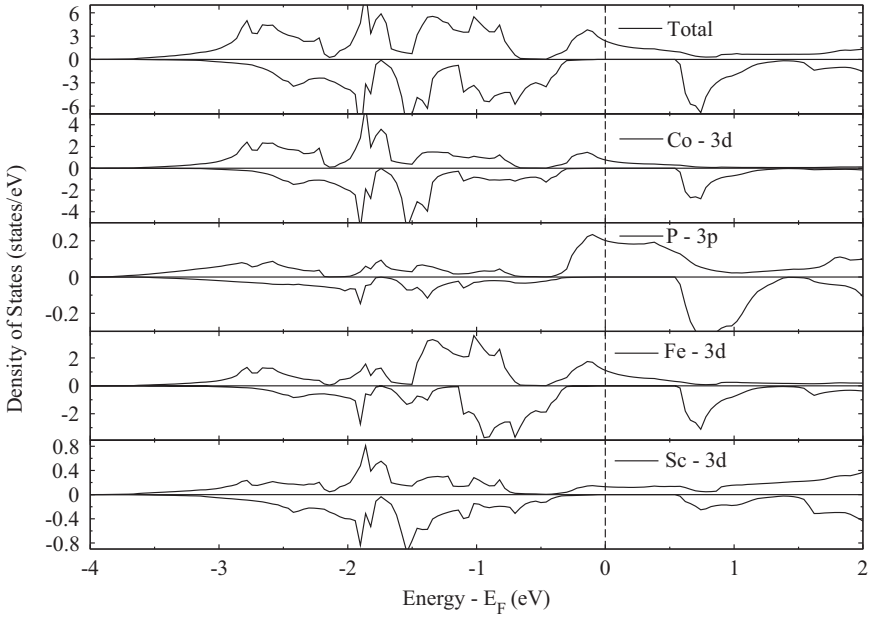

Fig. 1. The calculation results of total and partial DOS plots for quaternary Heusler alloy CoFeScP in Y-type (I) structure. The zero energy value is in correspondence to the Fermi level. Positive values of DOS represent spin-up electrons, while negative values represent spin-down electrons.